JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **8** No 4(1), 04029(3pp) (2016)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **8** № 4(1), 04029(3cc) (2016)

Semiholographic Approach in Calculation of Tunneling Current in Graphene with Deep Impurities

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(Received 18 June 2016; revised manuscript received 22 November 2016; published online 29 November 2016)

In this paper, we investigated the influence of deep impurity in graphene on the tunneling current in the contact with a metal. A ballistic current in graphene was calculated. The dependence of current-voltage characteristic of the contact on transition energy between the impurity and the graphene was analyzed.

Keywords: Tunneling current; Deep impurity; Semiholographic approach.

DOI: 10.21272/jnep.8(4(1)).04029 PACS numbers: 73.20. At, 73.22.Pr

1. INTORDUCTION

In this paper, we study the tunneling current in the contact of the graphene with deep impurities and metal. The term “deep impurity” used here refers to the impurity whose levels are lied above Fermi level and separated from the Fermi level on the value more kT [1]. The study of the materials with deep impurities is very important because such impurities have a great influence on the electronic structure — and thus the properties of semiconductors [2, 3].

The tunneling current of carbon nanotube with a metal without taking into account transitions between impurity levels was calculated in [4]. In this study, we take into account the transition to assess its degree of influence on the tunnel and an electric current, and do it in the framework of the semiholographic approach. Recently there are many researches in which ideas from both superstring theory and quantum gravitation find a use in condensed matter physics [5, 6]. So-called semiholographic approach was proposed recently as generalization of AdS/CFT correspondence ideas and holographic approach [7]. The main idea of the approach lies in the fact that graphene is described by dispersion law taken from the AdS/CFT correspondence, and interacting system is described by common way, for example, Green's function method. In this approach specific dispersion law of elementary excitations used in seed Green’s functions remains in holographic description of graphene. From this point of view, the approach is advanced enough since the holographic description of fermions is applied in different fields of solid state physics.

Initially, this approach proved to be very promising in the physics of systems with strongly correlated fermions [8, 9]. This method allows us to describe many of the observed dependence, in particular, the dependence of specific conductivity. At first glance, it seems that in graphene is irrelevant, since it is commonly used approximation of free fermions. However, in recent years there are many modifications of graphene, which can not be considered free fermions (even the discovery of the superconductivity effect in graphene). In this way, we have proposed approach looks promising. A case of common graphene we can obtain from this method if we annihilate the corresponding parameter in the proposed Green`s function.

Also, it should be noted that in recent years there are many works about practical application of carbon nanomaterials (nanotubes, graphene), including as a component of various types of devices [10-11], which action is based on the tunnel effect. In addition to the carbon nanostructure devices used as light sources [12], there are various kinds of devices based on the tunnel contact of nanotubes with different conductivity type [13].

2. STATEMENT OF THE PROBLEM AND BASIC EQUATIONS

We consider the graphene with double level impurity. Hamiltonian operator for this media can be written in matrix form as follows:

$$H = \begin{pmatrix} \varepsilon(k) & W_1 & W_2 \\ W_1^* & \varepsilon_1 & 0 \\ W_2^* & 0 & \varepsilon_2 \end{pmatrix}$$

ε_1, ε_2 are impurity levels, W_1, W_2 are constants of electron transition from impurity levels to condition in graphene, $\varepsilon(k)$ is the electron dispersion law for graphene, in particular for doped graphene.

Here, the Hamiltonian is defined in the wave function space $\begin{vmatrix} \psi_{fl} \\ \psi_1 \\ \psi_2 \end{vmatrix}\rangle$, where ψ_{fl} describes the electron wave function in graphene, ψ_1 corresponds to the wave function of the electron localized on the first level, ψ_2 corresponds to the wave function of the electron localized on the second level.

An exitatiob spectrum can be found with standart method, from condition $\det|H - \omega I| = 0$. Then we obtain the equation for eigenvalues:

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$$\omega^3-\omega^2\left(\varepsilon_1+\varepsilon_2+\varepsilon\right)+\omega\left(\varepsilon_1\varepsilon_2+\varepsilon\varepsilon_1+\varepsilon\varepsilon_2-\left|W_1\right|^2-\left|W_2\right|^2\right)+$$
$$+\left|W_1\right|^2\varepsilon_2+\left|W_2\right|^2\varepsilon_1-\varepsilon\varepsilon_1\varepsilon_2=0$$

Using the following replacement:

$$y=\omega-\frac{\varepsilon_1+\varepsilon_2+\varepsilon}{3}$$

we have three roots of the equation:

$$y_1=-2d\cos\left(\frac{\phi}{3}\right),\ y_2=2d\cos\left(\frac{\pi+\phi}{3}\right),\ y_3=2d\cos\left(\frac{2\pi+\phi}{3}\right),\ d=-\sqrt{|p|},$$
$$2q=\frac{-2\left(\varepsilon+\varepsilon_1+\varepsilon_2\right)^3}{27}+\frac{\left(\varepsilon+\varepsilon_1+\varepsilon_2\right)\left(\varepsilon_1\varepsilon_2+\varepsilon\varepsilon_1+\varepsilon\varepsilon_2-\left|W_1\right|^2-\left|W_2\right|^2\right)}{3}+$$
$$+\left|W_1\right|^2\varepsilon_2+\left|W_2\right|^2\varepsilon_1-\varepsilon\varepsilon_1\varepsilon_2$$
$$3p=\frac{3\left(\varepsilon_1\varepsilon_2+\varepsilon\varepsilon_1+\varepsilon\varepsilon_2-\left|W_1\right|^2-\left|W_2\right|^2\right)-\left(\varepsilon+\varepsilon_1+\varepsilon_2\right)^2}{3}$$

Further, we should take into account that the dispersion law for stimulation close to Fermi level in the framework of holographic approach is given by formula [7, 14]:

$$\omega=\varepsilon\left(k\right)+r\cdot\omega^{\gamma},$$
$$\varepsilon\left(k\right)=v_F\sqrt{k_x^2+k_y^2},$$
$$\gamma=2\Delta_k-1$$

where k_x, k_y are the pulse components, Δ_k is the conformal dimension, $r=\text{const}$ [15, 16]. The case of the common graphene corresponds to $r=0$.

In the case $\gamma=2$ we can obtain the dispersion law for doped graphene explicitly from ADS/CFT correspondence:

$$\omega=\frac{-1\pm\sqrt{1+4rv_F\sqrt{k_x^2+k_y^2}}}{2r}$$

Further, we choose positive sign.

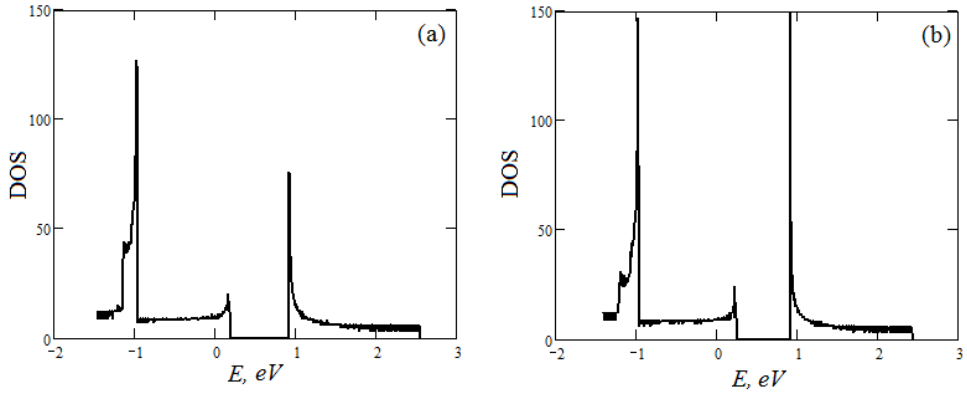

Fig. 1 – Electron density of states for graphene with deep impurity: (a) $\varepsilon_1 = 0.5$ eV, $\varepsilon_2 = 0.6$ eV; (b) $\varepsilon_1 = 0.7$ eV, $\varepsilon_2 = 0.8$ eV

The peaks correspond to the impurity levels.

3. TUNNELING AND BALLISTIC CURRENT

In the framework of Kubo theory, formula for the current density of the contact can be written in the following form [17]:

$$J_{tun}=4\pi e\left|T\right|^2\int_{-\infty}^{\infty}dE\nu_A(E+eV)\nu_B(E)(n_f(E)-n_f(E+eV))$$
$$\nu_A(E)=\sum_p\delta(E-E_p^A);\nu_B(E)=\sum_q\delta(E-E_q^B);\quad(5)$$

where $\delta(x)$ is the Dirac delta function, $\nu_{A(B)}(E)$ is the tunneling density of states; $n_f(E)$ is the equilibrium number of fermions with energy E. The approximation of a "rough" contact is hereinafter used, so that $T_{pq}=T$ (this imposes certain restrictions on the contact geometry, that is for the case discussed below means that graphene plane should be perpendicular to the contact material surface). For definiteness we choose the dispersion law for the graphene with deep impurities λ, and the dispersion law for the metal as the contact material being:

$$E_q^A=\frac{p^2}{2m},\quad(6)$$

After calculating the integrals in (5), it is easy to obtain tunneling current in the contact (Fig. 2).

As can be seen from Fig.4 increasing of the impurity energy result in an increasing of the electric current. The influence of the transition parameter between the impurity and graphene levels in the following ways: a closer transition energy for two levels to each other causes a reduction in the electric current. Thus, such current is also very suitable for the determination of the impurity and its concentration. As can be seen from the graphs, we have a noticeable impact of the impurity energy on the tunneling current in the system. Increasing of the impurity energy leads to increasing of the tunneling current, wherein the section with a negative differential conductance (NDC) does not change.

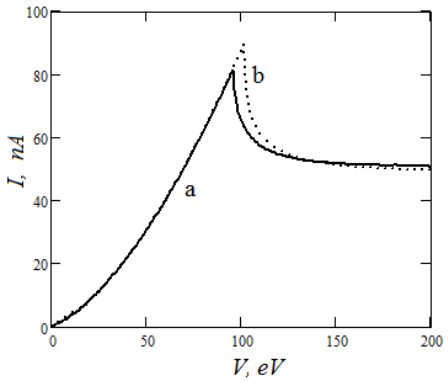

Fig. 2 – Dependence of tunneling current on voltage for the graphene-metal contact for the different values of impurity energy: (a) $\varepsilon_1 = 0.5$ eV, $\varepsilon_2 = 0.6$ eV; (b) $\varepsilon_1 = 0.7$ eV, $\varepsilon_2 = 0.8$ eV

Early we observed similar behavior in the study of the tunneling current in contact of a metal with graphene nanoribbons with multi-level impurities. Thus, it becomes possible to determine what kind of impurity adsorbed on graphene.

Ballistic current in graphene can be found by the formula [18] (Fig. 3):

$$J_{bal} = \frac{2e}{h}\int R(E)M(E)\big(f(E)-f(E+eV)\big)dE\,, \qquad (7)$$

here $T \approx \lambda_{sd}/(\lambda_{sc} + L)$, λ_{sc} is the scattering length, L is the sample length. The number of modes M is determined by the density of states, $f(E)$ is the Fermi distribution.

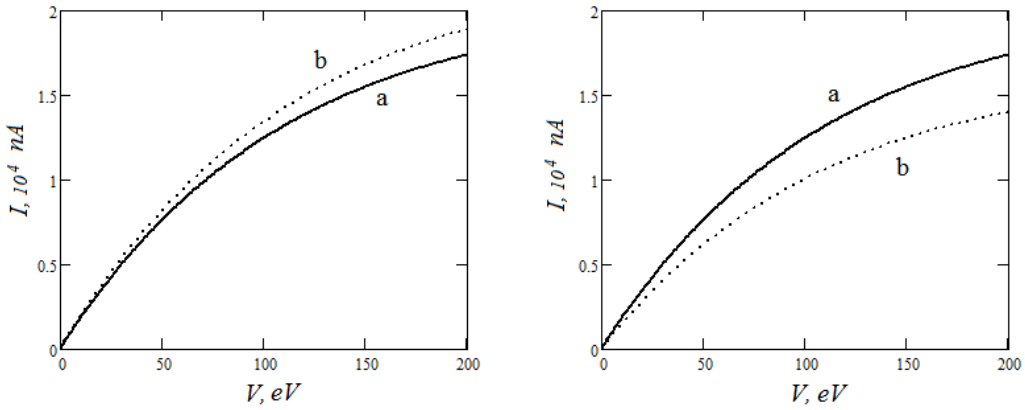

Fig. 3 – Dependence of ballistic current on voltage for graphene with deep impurity: A – for the different values of impurity energy: (a) $\varepsilon_1 = 0.5$ eV, $\varepsilon_2 = 0.6$ eV; (b) $\varepsilon_1 = 0.7$ eV, $\varepsilon_2 = 0.8$ eV; B – for the different values of transition energy: (a) $W_1 = 0.7$ eV, $W_2 = 0.3$ eV; (b) $W_1 = 0.6$ eV, $W_2 = 0.4$ eV

4. CONCLUSION

1. In the framework of semiholographic approach, the influence of impurity on the tunneling characteristic of the graphene-metal contact was studied.

2. The influence of impurity levels energy and transition energy from impurity levels to graphene on the current-voltage characteristic was shown.

It was revealed, that tunneling current as well as a common electrical current is sensitive to impurity. In the case when impurity levels energy increases, the tunneling current is also increases, as well as ballistic current. This fact can be associated with the changing of the state density of the sample.

This work was supported by the Russian Foundation for Basic Research under projects No. 16-32-00230 мол_а, No. 16-07-01265 А.

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